Data Evaluation Report on the adsorption-desorption of chlormequat chloride in soil

PMRA Submission Number {.....} EPA MRID Number 46715229

Data Requirement: PMRA Data Code:
EPA DP Barcode: D325184
OECD Data Point:
EPA Guideline: 163-1

Test material:

Common name: Chlormequat chloride.

Chemical name:

IUPAC name: 2-Chloroethyltrimethylammonium chloride.

CAS name: 2-Chloro-N,N,N-trimethylethanaminium chloride.

CAS No.: 999-81-5.

Synonyms Cycocel.

Smiles string: CN(C)(C)CCCl.[Cl-] (ISIS v2.3/Universal SMILES).
ClCCN(Cl)(C)(C)C (EPI Suite, v3.12).

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Company Code:
Active Code:
Use Site Category:
EPA PC Code: 018101

CITATION: Morgenroth U. 1995. Adsorption/desorption of ^{14}C-chlormequat-chloride on three soils. Unpublished study performed by RCC Umweltchemie AG, Itingen, Switzerland; sponsored and submitted by BASF Corporation, Research Triangle Park, NC.. Report Number 365545. BASF Registration Document Number 1998/10560. Experiment start date March 3, 1994, and completion date January 3, 1995 (p. 13). Final report issued August 03, 1995.

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EXECUTIVE SUMMARY

The adsorption/desorption characteristics of [chlorocholine-1,2-^{14}C]-labeled 2-chloroethyl-trimethylammonium chloride (chlormequat chloride) were studied in a sandy loam soil [pH 7.1, organic carbon 2.4%) and a loam soil [pH 7.2, organic carbon 1.0%], each from The Netherlands, and a silt loam soil [pH 7.4, organic carbon 2.1%] from Switzerland, in a batch equilibrium experiment. The experiment was conducted in accordance with OECD Guideline for Testing of Chemicals No. 106: "Adsorption/Desorption", and in compliance with USEPA FIFRA Title 40 CFR Part 160. The adsorption phase of the study was carried out by equilibrating air-dried soil with [^{14}C]chlormequat chloride at nominal test concentrations of 0.2, 1.0, 5.0, and 25.0 mg a.i./kg soil in the dark at 10 ± 1°C for 16 hours for the Breda sandy loam and Westmaas loam soils, and 5 hours for the Itingen silt loam soil. The equilibrating solution used was 0.01M $CaCl_2$ solution, with soil/solution ratios of 1:5 (w:v). The desorption phase of the study was carried out by replacing the adsorption solution with an equivalent volume of 0.01M $CaCl_2$ solution and equilibrating in the dark at 10 ± 1°C for 16 hours for the Breda sandy loam and Westmaas loam soils, and 17 hours for the Itingen silt loam soil. Two desorption steps were conducted for each test soil.

The supernatant solutions after adsorption and each desorption step were separated by centrifugation, and duplicate aliquots were analyzed for total radioactivity using LSC. Following adsorption, the high-dose soils (25.0 mg a.i./kg soil) were extracted three times with methanol:water (1:1, v:v), separated by centrifugation, and duplicate aliquots were analyzed for total radioactivity using LSC. Following the adsorption and desorption phases, duplicate aliquots of the soils were combusted and analyzed for total radioactivity using LSC. Aliquots of the high-dose adsorption supernatants were analyzed for [^{14}C]chlormequat chloride using TLC.

The incubation temperature during the study was reported to be maintained at 10 ± 1EC; supporting data were not provided. The pH of the test solutions during the study was not reported. [^{14}C]Chlormequat chloride accounted for all of the recovered radioactivity in the high-dose adsorption supernatants, based on TLC analysis.

Mass balances at the end of the adsorption phase averaged 99.7 ± 2.9% (range 97.6-101.7%), 97.7 ± 0.4% (range 97.4-98.0%), and 105.5 ± 2.5% (range 103.8-107.3%) of the applied for the high-dose Breda sandy loam, Westmaas loam, and Itingen silt loam soils, respectively. Mass balances following desorption were not determined.

After 5 or 16 hours of equilibration, 22.4-49.0%, 59.9-76.9%, and 58.1-63.5% of the applied [^{14}C]chlormequat chloride was adsorbed to the Breda sandy loam, Westmaas loam, and Itingen silt loam soils. Registrant-calculated Freundlich adsorption K values were 2.14, 9.12, and 8.08 for the Breda sandy loam, Westmaas loam, and Itingen silt loam soils, respectively; corresponding adsorption K_{oc} values were 89.35, 912.11, and 384.85. Following the second desorption step, the percent of [^{14}C]chlormequat chloride desorbed from the test soils, as percent of the radioactivity adsorbed, was 40.6-68.8% for the Breda sandy loam, 21.9-34.6% for the Westmaas loam, and 20.7-55.0% for the Itingen silt loam soils. Registrant-calculated Freundlich

desorption K values were 3.18, 12.49, and 10.78 for the Breda sandy loam, Westmaas loam, and Itingen silt loam soils, respectively; corresponding desorption K_{oc} values were 132.67, 1248.50, and 513.39.

Results Synopsis:

Soil type: Breda Sandy loam

Amount adsorbed:	22.4-49.0% of the applied.
Freundlich adsorption K:	2.14
Freundlich adsorption K_{oc}:	89.35
Amount desorbed:	40.6-68.8%
Freundlich desorption K:	3.18
Freundlich desorption K_{oc}:	132.67

Soil type: Westmaas Loam

Amount adsorbed:	59.9-76.9% of the applied.
Freundlich adsorption K:	9.12
Freundlich adsorption K_{oc}:	912.11
Amount desorbed:	21.9-34.6%
Freundlich desorption K:	12.49
Freundlich desorption K_{oc}:	1248.50

Soil type: Itingen Silt loam

Amount adsorbed:	58.1-63.5% of the applied.
Freundlich adsorption K:	8.08
Freundlich adsorption K_{oc}:	384.85
Amount desorbed:	20.7-55.0%
Freundlich desorption K:	10.78
Freundlich desorption K_{oc}:	513.39

Study Acceptability: This study is classified as **acceptable**. No significant deviations from good scientific practices were noted. It could not be determined if The Netherlands and Swiss soils were comparable to soils found in typical use areas in the United States. Material balances were determined only for high-dose soils following the adsorption phase. In addition, the experimental temperature was outside of the range of normal environmental parameters (18-30EC).

I. MATERIALS AND METHODS

GUIDELINE FOLLOWED: This study was conducted in accordance with OECD Guideline for Testing of Chemicals No. 106: "Adsorption/Desorption" (1981; p. 14). The following

significant deviations from the objectives of Subdivision N guidelines were noted:

It could not be determined if the foreign soils that were used in the study were typical of the pesticide use area in the US.

Material balances were determined for high-dose soils following the adsorption phase only.

The experimental temperature (10EC) was outside the range of normal environmental parameters (18-30EC).

COMPLIANCE: This study was conducted in compliance with USEPA FIFRA Good Laboratory Practice Standards Title 40 CFR Part 160 (1989), OECD GLP (1981); and Swiss GLP (1986; pp. 3-5). Signed and dated No Data Confidentiality, GLP, and Quality Assurance statements were provided (pp. 2-7). A Certificate of Authenticity was not provided.

A. MATERIALS:

1. Test Material [Chlorocholine-1,2-^{14}C]chlormequat chloride (p. 19).

Chemical Structure: See DER Attachment 1.

Description: Technical grade (radiolabeled test material).
Liquid, white to yellowish (unlabeled test material; p. 20).

Purity:

Radiolabeled

Radiochemical purity: 100.0% (pp. 19, 22; Figure 1, p. 51).
Batch No.: 93211.
Analytical purity: Not reported.
Specific radioactivity: 15.00 mCi/mmol (94.60 µCi/mg).
Location of the label: 1 and 2 carbons of the ethyl group.

Unlabeled

Analytical purity: 100.3% (p. 20).
Batch No.: WH 129(RS-0044).

Storage conditions of test chemicals: Radiolabeled test material was stored frozen (*ca.* -20°C) in the dark (p. 19). Unlabeled test material was stored in the original container protected from light and under cool, dry conditions (p. 20).

Physico-chemical properties of chlormequat chloride

Parameter	Value	Comment
Molecular weight	158.56 g/mole 158.1 g/mole	Radiolabeled test material. Unlabeled test material.
Molecular formula	$C_5H_{13}Cl_2N$	
Water Solubility	10^6 mg/L	At 20°C.
Vapor Pressure/Volatility	Not reported.	
UV Absorption	Not reported.	
Pka	Not reported.	
K_{ow}/log K_{ow}	Not reported.	
log P_{ow}	Not reported.	
Stability of compound at room temperature, if provided	Not reported.	

Data were obtained from pp. 19-20 of the study report.

2. Soil Characteristics

Table 1: Description of soil collection and storage.

Description	Breda Sandy loam	Westmaas Loam	Itingen Silt loam
Geographic location	Site 22, The Netherlands	Site 1, The Netherlands	Switzerland
Pesticide use history at the collection site	Not reported.		None for previous 3 years.
Collection procedures	Samples were collected from 1 or more places within the field plot.		Not reported.
Sampling depth	15-20 cm		*ca.* 30 cm
Storage conditions	Stored in open plastic bags under aerobic conditions.		Not reported.
Storage length [1]	*ca.* 10 months.		*ca.* 33 months.
Soil preparation	Air-dried and sieved (<2mm).		Air-dried and sieved (<2mm).

Data were obtained from pp. 17-18 of the study report.

1 The storage length was determined by the reviewer as the interval from soil collection (May 1993 for The Netherlands soils, June 1991 for the Swiss soils) to experimental study initiation (March 1994).

Table 2: Properties of the soils.

Property	Breda	Westmaas	Itingen
Soil texture (USDA)	Sandy loam	Loam	Silt loam
% Sand (>50 µm)	73.7	33.5	21.1
% Silt (2-50 µm)	14.0	47.5	72.4
% Clay (<2 µm)	12.3	19.0	6.5
pH (KCl)	7.1	7.2	7.4
Organic carbon (g/100 g soil)%	2.4	1.0	2.1
Organic matter (%) [1]	4.1	1.7	3.6
CEC (meq/100 g soil)	14.8	17.9	31.2
$CaCO_3$ (%)	Not reported.		
Moisture at 1/3 atm (%)	Not reported.		
Field capacity (%)	Not reported.		
Maximum water holding capacity (%)	Not reported.		
Bulk density (g/cm^3)	Not reported.		
Biomass (mg microbial C/100 g or CFU or other)	Not reported.		
Soil taxonomic classification	Not reported.		
Soil mapping unit (for EPA)	Not reported.		

Data were obtained from p. 17 of the study report.
1 Reviewer-calculated as % organic carbon × 1.72.

C. STUDY DESIGN:

1. Preliminary study: A preliminary experiment was conducted to determine the appropriate equilibrium time to be used in the definitive study (pp. 22-23).

To determine the appropriate equilibration time to be used in the definitive study, duplicate Teflon tubes for the Breda sandy loam and Westmaas loam soils were prepared containing 5.0-g (dry weight equivalent) aliquots of soil and duplicate Teflon tubes for the Itingen silt loam soil were prepared containing 5.3-g (moist weight) aliquots of soil (pp. 21, 23). Each sample was mixed with a 25-mL aliquot of a 0.01M $CaCl_2$ solution containing [^{14}C]chlormequat chloride. The samples were shaken in the dark at 10 ± 1°C. Following 1, 2, 4, 6, and 24 hours of equilibration for the Breda sandy loam and Westmaas loam soils and 1, 2, 4, 6, and 22 hours for the Itingen silt loam soil, the samples were centrifuged and duplicate aliquots were analyzed for total radioactivity using LSC. Additional samples were analyzed using TLC. The amount of radioactivity adsorbed to the test containers was determined by calculating the difference between total amount of test article applied and the amount found in the supernatant. It was determined that the test soils reached equilibrium after 2 hours of incubation, with 22.7-60.3% of the applied [^{14}C]chlormequat chloride adsorbing to all test soils (Table 1, p. 39; Figure 3, p. 53). Based on TLC analysis, it was shown that [^{14}C]chlormequat chloride was stable in the test systems for up to 24 hours. Based on these results, it was determined that the definitive study

would be conducted using an equilibration time of 16 hours for the Breda sandy loam and Westmaas loam soils and 5 hours for the Itingen silt loam soil.

2. Definitive study experimental conditions:

Table 3: Study design for the adsorption phase.

Parameters		Breda Sandy loam	Westmaas Loam	Itingen Silt loam
Condition of soil (air dried/fresh) [1]		Air-dried.		
Have these soils been used for other laboratory studies? (specify which)		No.		
Soil (g/replicate)		5.0 g (dry weight equivalent).	5.0 g (dry weight equivalent).	5.3 g (wet soil).
Equilibrium solution used (eg: 0.01N $CaCl_2$)		0.01M $CaCl_2$		
Control used (with salt solution only) (Yes/No)		Yes		
Test material concentrations [2]	Nominal application rates (mg a.i./kg soil)	0.2, 1.0, 5.0, 25.0		
	Analytically measured concentrations (mg a.i./kg soil)	0.2-0.21, 1.005-1.035, 5.05-5.105, 25.13-25.585 (Breda/Westmass) 0.189-0.198, 0.948-0.976, 4.764-4.816, 23.707-24.136 (Itingen)		
Identity and concentration of co-solvent, if any		Methanol, *ca.* 1% by volume.		
Soil:solution ratio		1:5 (w:v)		
Initial pH of the equilibration solution, if provided		Not reported.		
No. of replications	Controls	2		
	Treatments	2		
Equilibration	Time (hours)	16	16	5
	Temperature (°C)	10 ± 1		
	Darkness (Yes/No)	Yes		
	Shaking method	Laboratory shaker.		
	Shaking time (hours)	16	16	5
Method of separation of supernatant (eg., centrifugation)		Centrifugation		
Centrifugation	Speed (rpm)	2000		
	Duration (min)	10		
	Method of separation of soil and solution	Decanted.		

Data were obtained from pp. 18, 21-24 of the study report.
1 The test soils were saturated with 0.01M $CaCl_2$ solution (2:1, vol:mass) over the weekend prior to use (p. 18).
2 Test material concentrations were calculated by the reviewer by converting mg/L to mg a.i./kg using the following equation: [test concentration (mg/L) × total volume of test material (mL)] ÷ amount of soil (g); eg. [0.04 mg/L × 25 mL] ÷5.0 g = 0.2 mg a.i./kg soil.

Table 4: Study design for the desorption phase.

Parameters		Breda Sandy loam	Westmaas Loam	Itingen Silt loam
Were the soil residues from the adsorption phase used? If not, describe the method for adsorption using a separate adsorption		Yes.		
Amount of test material present in the adsorbed state/adsorbed amount (mg a.i./kg soil)	0.2	0.10	0.15	0.14
	1.0	0.41	0.74	0.65
	5.0	1.54	3.36	3.09
	25.0	5.63	15.05	14.87
No. of desorption cycles		2		
Equilibration solution and quantity used per treatment for desorption (eg., 0.01M $CaCl_2$)		0.01M $CaCl_2$; 25 mL.		
Soil:solution ratio		1:5 (w:v).		
Replications	Controls	2		
	Treatments	2		
Desorption equilibration	Time (hours)	16	16	17
	Temperature (°C)	10 ± 1		
	Darkness	Yes		
	Shaking method	Laboratory shaker.		
	Shaking time (hours)	16	16	17
Centrifugation	Speed (rpm)	2000		
	Duration (min)	10		
	Method of separation of soil and solution	Decanted.		
Second desorption cycle		Same for the sandy loam and loam soils. For the silt loam soil, the second desorption step lasted 24 hours.		

Data were obtained from pp. 21-24 and Tables 2-3, pp. 40-41 of the study report.

3. Description of analytical procedures:

Extraction/clean up/concentration methods: Following adsorption, the high-dose soils (25.0 mg a.i./kg soil) were extracted three times with methanol:water (1:1, v:v; 20 mL) at pH 2 followed by centrifugation at 1500 rpm (p. 24).

Total ^{14}C measurement: Following adsorption and each desorption step, duplicate aliquots (up to 0.5 mL) of the supernatants were analyzed for total radioactivity using LSC (p. 25). Following extraction, duplicate aliquots (up to 0.5 mL) were analyzed for total radioactivity using LSC. Mass balances were determined for high-dose soils only, by summing the radioactivity recovered from the adsorption supernatants, organic extracts, and unextracted radiocarbon (p. 24).

Non-extractable residues, if any: Following adsorption and desorption, duplicate aliquots of the soils were combusted and analyzed for total radioactivity using LSC (pp. 24-25). Combustion efficiencies were not reported.

Derivatization method, if used: A derivatization method was not employed in this study.

Identification and quantification of parent compound: Aliquots of the high-dose adsorption supernatants were analyzed for [^{14}C]chlormequat chloride using TLC analysis on pre-coated Cellulose F, No. 5728 plates (5 × 20 cm, 20 × 20 cm; 0.25 mm thickness) developed in n-butanol:acetic acid:water (4:1:5, v:v:v; SS 1) and n-butanol:ethanol:acetic acid:water (8:2:1:3, v:v:v:v; SS 3; pp. 24, 26). Following development, areas of radioactivity were detected and quantified using a TLC Linear Analyzer. Unlabeled reference compounds were visualized by spraying with a 1% solution of molybdatophosphoric acid in ethanol:chloroform (1:1, v:v), rinsing with water, and spraying with a 1% solution of stannous-II-chloride in 3N HCl so that quaternary amines appeared as blue spots. Rf values for unlabeled chlormequat chloride were 0.48 (SS 1) and 0.53 (SS 3).

Identification and quantification of transformation products, if appropriate: Samples were not analyzed for transformation products of chlormequat chloride.

Detection limits (LOD, LOQ) for the parent compound: Limits of Detection (LOD) and Limits of Quantification (LOQ) were not reported.

Detection limits (LOD, LOQ) for the transformation products, if appropriate: Samples were not analyzed for transformation products of chlormequat chloride.

II. RESULTS AND DISCUSSION

A. TEST CONDITIONS: The experimental temperature employed during the study was reported to be maintained at 10 ± 1EC; supporting data were not provided (p. 21). The pH of the test solutions during the study was not reported. Based on TLC analysis of the high-dose adsorption supernatants, [^{14}C]chlormequat chloride accounted for all of the recovered radioactivity (p. 34; Figures 7-9, pp. 57-59).

B. MASS BALANCE: Mass balances at the end of the adsorption phase averaged 99.7 ± 2.9% (range 97.6-101.7%), 97.7 ± 0.4% (range 97.4-98.0%), and 105.5 ± 2.5% (range 103.8-107.3%) of the applied for the high-dose Breda sandy loam, Westmaas loam, and Itingen silt loam soils, respectively (p. 34; Table 5, p. 43). Mass balances at the end of the desorption phase were not determined.

Table 5: Recovery of [^{14}C]chlormequat chloride, expressed as percentage of applied radioactivity, in high-dose soil after adsorption/desorption (mean ± s.d.).

Matrices	Breda Sandy loam	Westmaas Loam	Itingen Silt loam
At the end of the adsorption phase			
Supernatant solution	72.6 ± 1.2	36.7 ± 0.2	37.9 ± 0.5
Solid phase (extracted) and Non-extractable residues in soil [1]	27.1 ± 1.7	61.0 ± 0.2	67.7 ± 3.0
Total recovery	99.7 ± 2.9	97.7 ± 0.4	105.5 ± 2.5
At the end of the desorption phase			
Supernatant solution	Not determined.		
Solid phase (^{14}C residues)	Not determined.		
Non-extractable residues in soil, if measured	Not determined.		
Total recovery	Not determined.		

Data were obtained from Table 5, p. 43 of the study report.
1 The soils were extracted prior to combustion. The study author reported the extraction and combustion values as a single sum.

Table 6: Concentration of [^{14}C]chlormequat chloride in the solid and liquid phases at the end of adsorption equilibration period (mean ± s.d.).

Concentration (mg a.i./kg soil)	Breda Sandy loam			Westmaas Loam		
	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed
0.2	0.10 ± 0.0	0.02 ± 0.0	49.0 ± 2.3	0.15 ± 0.0	0.01 ± 0.0	76.9 ± 0.0
1.0	0.41 ± 0.0	0.11 ± 0.0	40.8 ± 0.4	0.74 ± 0.0	0.05 ± 0.0	73.3 ± 0.4
5.0	1.54 ± 0.0	0.65 ± 0.0	30.4 ± 0.7	3.36 ± 0.0	0.31 ± 0.0	66.5 ± 0.7
25.0	5.63 ± 0.0	3.59 ± 0.0	22.4 ± 0.1	15.05 ± 0.2	1.84 ± 0.0	59.9 ± 0.8

Concentration (mg a.i./kg soil)	Itingen Silt loam		
	on soil (mg a.i./kg)	In solution (µg a.i./mL)	% adsorbed
0.2	0.14 ± 0.0	0.01 ± 0.0	63.5 ± 1.3
1.0	0.65 ± 0.0	0.07 ± 0.0	62.4 ± 3.1
5.0	3.09 ± 0.1	0.36 ± 0.0	60.5 ± 1.3
25.0	14.87 ± 0.4	1.93 ± 0.1	58.1 ± 1.5

Data were obtained from Tables 2-3, pp. 40-41 and Tables 7-9, pp. 45-47 of the study report. Means and standard deviations were determined by the reviewer using Excel.

Table 7a: Concentration of [^{14}C]chlormequat chloride in the solid and liquid phases at the end of first desorption step.

Concentration (mg a.i./kg soil)	Breda Sandy loam			Westmaas Loam		
	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% desorbed as % of the adsorbed	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% desorbed as % of the adsorbed
0.2	0.07 ± 0.0	0.01 ± 0.0	ND	0.13 ± 0.0	0.01 ± 0.0	ND
1.0	0.27 ± 0.0	0.04 ± 0.0	ND	0.61 ± 0.0	0.03 ± 0.0	ND
5.0	0.88 ± 0.1	0.18 ± 0.0	ND	2.72 ± 0.0	0.16 ± 0.0	ND
25.0	2.68 ± 0.1	0.83 ± 0.0	ND	11.2 ± 0.1	0.94 ± 0.0	ND

Concentration (mg a.i./kg soil)	Itingen Silt loam		
	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% desorbed as % of the adsorbed
0.2	0.12 ± 0.0	0.01 ± 0.0	ND
1.0	0.55 ± 0.0	0.03 ± 0.0	ND
5.0	2.42 ± 0.1	0.18 ± 0.0	ND
25.0	10.87 ± 0.0	1.02 ± 0.1	ND

Data were obtained from Tables 10-11, pp. 48-49 of the study report. Means and standard deviations were determined by the reviewer using Excel.
ND = Not determined.

Table 7b: Concentration of [^{14}C]chlormequat chloride in the solid and liquid phases at the end of second desorption step.[1]

Concentration (mg a.i./kg soil)	Breda Sandy loam			Westmaas Loam		
	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% desorbed as % of the adsorbed	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% desorbed as % of the adsorbed
0.2	ND	ND	40.56	ND	ND	21.92
1.0	ND	ND	49.03	ND	ND	25.03
5.0	ND	ND	58.16	ND	ND	26.06
25.0	ND	ND	68.76	ND	ND	34.59

Concentration (mg a.i./kg soil)	Itingen Silt loam		
	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% desorbed as % of the adsorbed
0.2	ND	ND	20.71
1.0	ND	ND	24.30
5.0	ND	ND	34.49
25.0	ND	ND	55.01

Data were obtained from Tables 7-9, pp. 45-47 of the study report.
1 Concentration data following the second desorption step were not provided.
ND = Not determined.

Table 8: Adsorption and desorption constants of [^{14}C]chlormequat chloride in the soils.

Soil	Adsorption						Desorption					
	K_d	K_F	1/N	r^2	K_{oc}	K_{Foc}	K_d	K_F	1/N	r^2	K_{oc}	K_{Foc}
Breda Sandy loam	NR	2.14	0.7680	0.9998	NR	89.35	NR	3.18	0.7629	0.9996	NR	132.67
Westmaas Loam	NR	9.12	0.8486	0.9999	NR	912.11	NR	12.49	0.8590	0.9996	NR	1248.50
Itingen Silt loam	NR	8.08	0.9553	1.0000	NR	384.85	NR	10.78	0.8618	0.9997	NR	513.39

Data were obtained from pp. 33, 35, Table 4, p. 42, Table 12, p. 50, and Figure 10, p. 60 of the study report.
K_d - Adsorption and desorption coefficients; K_F - Freundlich adsorption and desorption coefficients; 1/N - Slope of Freundlich adsorption/desorption isotherms.
K_{oc} - Coefficient adsorption per organic carbon (K_d or K x 100/% organic carbon).
r^2 - Regression coefficient of Freundlich equation.
NR = Not reported.

C. ADSORPTION: After 5 or 16 hours of equilibration, 22.4-49.0%, 59.9-76.9%, and 58.1-63.5% of the applied [^{14}C]chlormequat chloride was adsorbed to the Breda sandy loam, Westmaas loam, and Itingen silt loam soils, respectively (Tables 7-9, pp. 45-47). Registrant-calculated adsorption K values were 2.14, 9.12, and 8.08 for the Breda sandy loam, Westmaas loam, and Itingen silt loam soils, respectively; corresponding adsorption K_{oc} values were 89.35, 912.11, and 384.85 (Table 4, p. 42). Registrant-calculated Freundlich adsorption K and K_{oc} values were not reported.

D. DESORPTION: Following the second desorption step, the percent of [^{14}C]chlormequat chloride desorbed from the test soils, as percent of the radioactivity adsorbed, was 40.6-68.8% for the Breda sandy loam, 21.9-34.6% for the Westmaas loam, and 20-7-55.0% for the Itingen silt loam soils (Tables 7-9, pp. 45-47). Registrant-calculated desorption K values were 3.18, 12.49, and 10.78 for the Breda sandy loam, Westmaas loam, and Itingen silt loam soils, respectively; corresponding desorption K_{oc} values were 132.67, 1248.50, and 513.39 (Table 12, p. 50). Registrant-calculated Freundlich desorption K and K_{oc} values were not reported.

III. STUDY DEFICIENCIES

1. It was not established that the foreign soils used in this study were comparable to soils that would be found at the intended use sites in the United States. The foreign test soils were from The Netherlands and Switzerland, and the FAO classifications were not provided.

2. Material balances were determined for high-dose soils following the adsorption phase only. Mass balances should have been determined for all test concentrations/test soil groups following adsorption and following desorption.

3. The experimental temperature (10EC) was outside the range of normal environmental parameters (18-30EC).

IV. REVIEWER'S COMMENTS

1. None of the test soils had an organic matter content #1%, as recommended by Subdivision N guidelines.

2. The Freundlich 1/n values for the adsorption phase for the Breda sandy loam and Westmaas loam soils, and desorption phase for all three test soils were below 0.9. Subdivision N guidelines specify that 1/n values should be in the range of 0.9 to 1.1.

3. [^{14}C]Chlormequat chloride had low mobility in the Westmaas loam and Itingen silt loam soils and medium mobility in the Breda sandy loam soil, based on the study results according to Hamaker (1975) (pp. 36-37).

4. [^{14}C]Chlormequat chloride was stable in solution before and after application, based on TLC analysis of the application solution (pp. 22, 32; Figure 2, p. 52).

5. To confirm adsorption constant data reported in the study report, the reviewer calculated adsorption K_d values using the following EPA-approved equation:

   $K_d = [(C_0V_0 - C_{eq}V_0) \div m] \div C_{eq}$ where

   S = the sorbed phase concentration with units of mass of sorbate per solid sorbent mass;
   C_0 = the concentration in the water before sorption;
   V_0 = the total water volume in the batch system;
   C_{eq} = the aqueous-phase equilibrium concentration; and
   m = the dry mass of sorbent.

   The results of these calculations are tabulated below:

Table 9: Reviewer-calculated adsorption constants of [^{14}C]chlormequat chloride in the soil.

Soil	K_d
Breda Sandy loam	3.48
Westmaas Loam	12.57
Itingen Silt loam	10.02

K_d values were reviewer-calculated using data obtained from Tables 2-3, pp. 40-41 of the study report.

The reviewer-calculated r^2 value for Kads vs. % organic carbon was 0.7116, Kads vs. pH was 0.3019, and Kads vs. % clay was 0.0971.

6. Limits of Detection and Limits of Quantification for LSC and TLC analysis were not reported. Limits of detection and limits of quantification should be reported to allow the reviewer to evaluate the adequacy of the test method for the determination of the parent compound and its transformation products.

7. The maximum field application rate for chlormequat chloride was not reported. Subdivision N guidelines specify that one test concentration should be roughly equivalent to the maximum proposed or registered field application rate of the parent compound.

V. REFERENCES

1. U.S. Environmental Protection Agency. 1982. Pesticide Assessment Guidelines, Subdivision N, Chemistry: Environmental Fate, Section 163-1. Mobility studies. Office of Pesticide and Toxic Substances, Washington, DC. EPA 540/9-82-021.

2. U.S. Environmental Protection Agency. 1989. FIFRA Accelerated Reregistration, Phase 3 Technical Guidance. Office of the Prevention, Pesticides, and Toxic Substances, Washington, DC. EPA 540/09-90-078.

3. U.S. Environmental Protection Agency. 1993. Pesticide Registration Rejection Rate Analysis - Environmental Fate. Office of the Prevention, Pesticides, and Toxic Substances, Washington, DC. EPA 738.

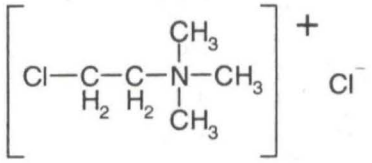
4. U.S. Environmental Protection Agency. 2003. Guidance for Calculating Sorption Coefficients in Batch Equilibrium Studies.

Attachment 1: Structures of Parent Compound and Transformation Products

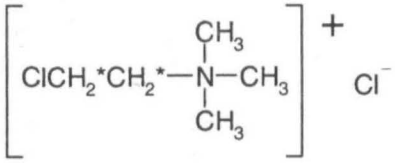
Chlormequat chloride [Cycocel]

IUPAC Name: 2-Chloroethyltrimethylammonium chloride.
CAS Name: 2-Chloro-N,N,N-trimethylethanaminium chloride.
CAS Number: 999-81-5.
SMILES String: CN(C)(C)CCCl.[Cl-] (ISIS v2.3/Universal SMILES).
ClCCN(Cl)(C)(C)C (EPI Suite, v3.12).

Unlabeled



[^{14}C]chlormequat chloride

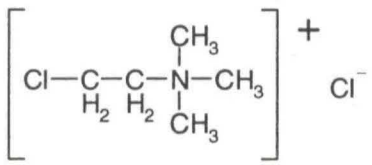


* = Position of radiolabel.

Identified Compounds

Chlormequat chloride [Cycocel]

IUPAC Name: 2-Chloroethyltrimethylammonium chloride.
CAS Name: 2-Chloro-N,N,N-trimethylethanaminium chloride.
CAS Number: 999-81-5.
SMILES String: CN(C)(C)CCCl.[Cl-] (ISIS v2.3/Universal SMILES).
ClCCN(Cl)(C)(C)C (EPI Suite, v3.12).



Attachment 2: Excel Spreadsheets

Chemical: Chlormequat chloride
PC Code: 018101
MRID: 46715229
Guideline No: 163-1

Table 4/6 Adsorption on soil

	Sandy loam	Loam	Silt loam
5	5.61	14.91	15.15
5	5.64	15.19	14.59
AVG	5.63	15.05	14.87
STDEV	0.02	0.20	0.40
1	1.56	3.33	3.04
1	1.51	3.38	3.13
AVG	1.54	3.36	3.09
STDEV	0.04	0.04	0.06
0.2	0.41	0.74	0.67
0.2	0.41	0.74	0.62
AVG	0.41	0.74	0.65
STDEV	0.00	0.00	0.04
0.04	0.10	0.15	0.13
0.04	0.09	0.15	0.14
AVG	0.10	0.15	0.14
STDEV	0.01	0.00	0.01

Data were obtained from Tables 2-3, pp. 40-41 of the study report.

Table 5 Adsorption phase- adsorption solution

	Sandy loam	Loam	Silt loam
5	71.70	36.54	37.53
5	73.40	36.86	38.18
AVG	72.55	36.70	37.86
STDEV	1.2	0.2	0.5

Table 5 Adsorption phase- extracted and combusted

	Sandy loam	Loam	Silt loam
5.37	25.90	60.87	69.76
5.37	28.32	61.12	65.57
AVG	27.11	61.00	67.67
STDEV	1.7	0.2	3.0

Table 5 Adsorption phase- recovery

	Sandy loam	Loam	Silt loam
5.37	97.60	97.41	107.29
5.37	101.72	97.98	103.75
AVG	99.66	97.70	105.52
STDEV	2.9	0.4	2.5

Data were obtained from Table 5, p. 43 of the study report.

Chemical: Chlormequate chloride
PC Code: 18101
MRID: 46715229
Guideline No: 163-1

Table 6 Adsorption in solution

	Sandy loam	Loam	Silt loam
5	3.61	1.86	1.87
5	3.57	1.81	1.98
AVG	3.59	1.84	1.93
STDEV	0.03	0.04	0.08
1	0.64	0.31	0.37
1	0.65	0.30	0.35
AVG	0.65	0.31	0.36
STDEV	0.01	0.01	0.01
0.2	0.11	0.05	0.07
0.2	0.11	0.05	0.07
AVG	0.11	0.05	0.07
STDEV	0.00	0.00	0.00
0.04	0.02	0.01	0.01
0.04	0.02	0.01	0.01
AVG	0.02	0.01	0.01
STDEV	0.00	0.00	0.00

Data were obtained from Tables 2-3, pp. 40-41 of the study report.

Table 6 % Adsorbed

	Sandy loam	Loam	Silt loam
5	22.32	59.33	59.21
5	22.44	60.43	57.04
AVG	22.38	59.88	58.13
STDEV	0.08	0.78	1.53
1	30.91	66.04	59.58
1	29.88	66.99	61.37
AVG	30.40	66.52	60.48
STDEV	0.73	0.67	1.27
0.2	40.59	73.56	64.54
0.2	41.09	73.06	60.18
AVG	40.84	73.31	62.36
STDEV	0.35	0.35	3.08
0.04	50.67	76.92	62.55
0.04	47.38	76.86	64.34
AVG	49.03	76.89	63.45
STDEV	2.33	0.04	1.27

Data were obtained from Tables 7-9, pp. 45-47 of the study report.

Chemical: Chlormequate chloride
PC Code: 18101
MRID: 46715229
Guideline No: 163-1

Table 7 Desorption on soil

	Sandy loam	Loam	Silt loam
5	2.58	11.16	10.90
5	2.77	11.24	10.84
AVG	2.68	11.20	10.87
STDEV	0.13	0.06	0.04
1	0.92	2.71	2.37
1	0.83	2.73	2.46
AVG	0.88	2.72	2.42
STDEV	0.06	0.01	0.06
0.2	0.27	0.61	0.57
0.2	0.26	0.61	0.52
AVG	0.27	0.61	0.55
STDEV	0.01	0.00	0.04
0.04	0.07	0.13	0.11
0.04	0.07	0.13	0.12
AVG	0.07	0.13	0.12
STDEV	0.00	0.00	0.01

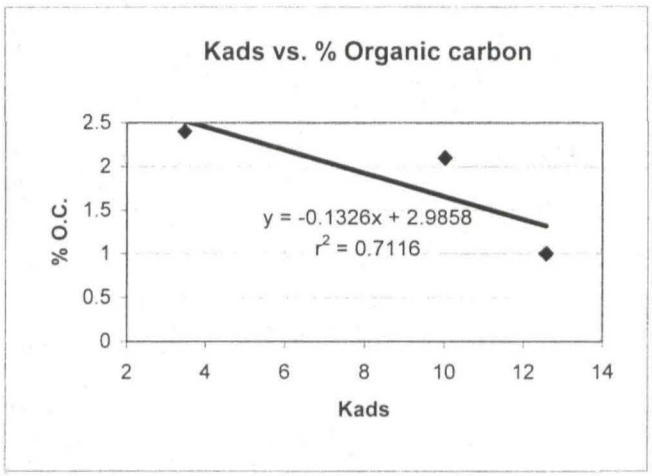
Table 7 Desorption in solution

	Sandy loam	Loam	Silt loam
5	0.83	0.93	1.07
5	0.83	0.94	0.97
AVG	0.83	0.94	1.02
STDEV	0.00	0.01	0.07
1	0.18	0.16	0.18
1	0.18	0.16	0.18
AVG	0.18	0.16	0.18
STDEV	0.00	0.00	0.00
0.2	0.04	0.03	0.03
0.2	0.04	0.03	0.03
AVG	0.04	0.03	0.03
STDEV	0.00	0.00	0.00
0.04	0.01	0.01	0.01
0.04	0.01	0.01	0.01
AVG	0.01	0.01	0.01
STDEV	0.00	0.00	0.00

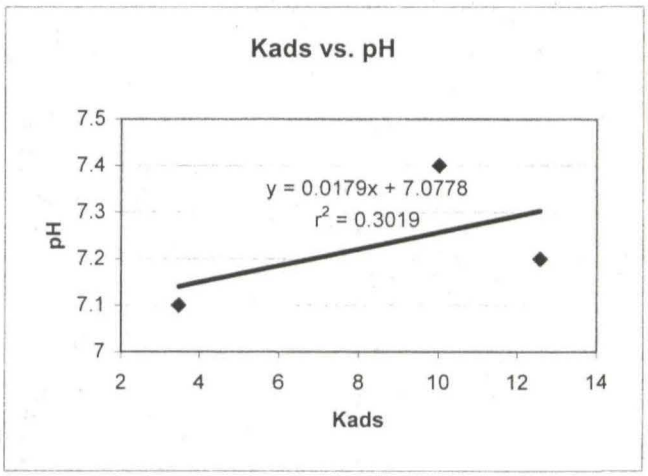
Data were obtained from Tables 10-11, pp. 48-49 of the study report.

Chemical: Chlormequat chloride
PC Code: 018101
MRID: 46715229
Guideline No: 163-1

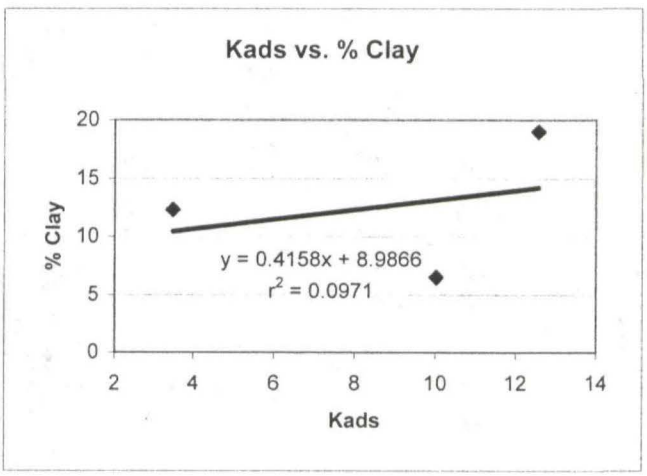
Soil	Kads	% organic carbon
Sandy loam	3.48	2.4
Loamy sand	12.57	1
Silt loam	10.02	2.1



Soil	Kads	pH
Sandy loam	3.48	7.1
Loamy sand	12.57	7.2
Silt loam	10.02	7.4



Soil	Kads	% clay
Sandy loam	3.48	12.3
Loamy sand	12.57	19
Silt loam	10.02	6.5



Data were obtained from p. 17. Kads values were reviewer-calculated using data obtained from Tables 2-3, pp. 40-41 of the study report.

Chemical: Chlormequat chloride
PC Code: 018101
MRID: 46715229
Guideline No: 163-1

Breda Sandy loam- Adsorption

Initial soln concen (C_o) (ug/mL)	Volume of soln (V_o) (mL)	Concen in soln after equil (C_{eq}) (ug/mL)	Volume of soln (V_o) (mL)	Dry mass of sorbent (m) (g)	$[(C_oV_o)-(C_{eq}V_o)]$/soil mass	Kd	
5.03	25	3.61	25	5	7.1000	1.97	
5.03	25	3.57	25	5	7.3000	2.04	
1.01	25	0.64	25	5	1.8500	2.89	
1.01	25	0.65	25	5	1.8000	2.77	
0.2	25	0.11	25	5	0.4500	4.09	
0.2	25	0.11	25	5	0.4500	4.09	
0.04	25	0.02	25	5	0.1000	5.00	
0.04	25	0.02	25	5	0.1000	5.00	
						3.48	AVG

Westmaas Loam- Adsorption

Initial soln concen (C_o) (ug/mL)	Volume of soln (V_o) (mL)	Concen in soln after equil (C_{eq}) (ug/mL)	Volume of soln (V_o) (mL)	Dry mass of sorbent (m) (g)	$[(C_oV_o)-(C_{eq}V_o)]$/soil mass	Kd	
5.03	25	1.86	25	5	15.8500	8.52	
5.03	25	1.81	25	5	16.1000	8.90	
1.01	25	0.31	25	5	3.5000	11.29	
1:01	25	0.3	25	5	3.5500	11.83	
0.2	25	0.05	25	5	0.7500	15.00	
0.2	25	0.05	25	5	0.7500	15.00	
0.04	25	0.01	25	5	0.1500	15.00	
0.04	25	0.01	25	5	0.1500	15.00	
						12.57	AVG

Itingen Silt loam- Adsorption

Initial soln concen (C_o) (ug/mL)	Volume of soln (V_o) (mL)	Concen in soln after equil (C_{eq}) (ug/mL)	Volume of soln (V_o) (mL)	Dry mass of sorbent (m) (g)	$[(C_oV_o)-(C_{eq}V_o)]$/soil mass	Kd	
5.12	25	1.87	25	5.3	15.3302	8.20	
5.12	25	1.98	25	5.3	14.8113	7.48	
1.02	25	0.37	25	5.3	3.0660	8.29	
1.02	25	0.35	25	5.3	3.1604	9.03	
0.21	25	0.07	25	5.3	0.6604	9.43	
0.21	25	0.07	25	5.3	0.6604	9.43	
0.04	25	0.01	25	5.3	0.1415	14.15	
0.04	25	0.01	25	5.3	0.1415	14.15	
						10.02	AVG

Data were obtained from Tables 2-3, pp. 40-41 of the study report.